



Classification No.: 2180.1

Approval Date: 6/26/87

CHEMICAL ABSTRACT SERVICE REGISTRY NUMBER DATA STANDARD

1. PURPOSE. This Order establishes the policy and responsibilities related to the use of registry data, specifically the Registry Number, from the Chemical Abstracts Service (CAS) Division of the American Chemical Society in automated information systems containing data/information on specific, definable chemical substances. The CAS registry number provides consistent and unambiguous identification of chemicals and facilitates sharing chemical information across programmatic media.
2. SCOPE AND APPLICABILITY. This data standard applies to all EPA organizations and their employees as well as the facilities and personnel of agents of EPA who design, develop, operate or maintain Agency information and information systems having to do with specific, definable chemical substances. It also applies to EPA contractors and assistance recipients.
3. REFERENCE.

Chapter 5 of the EPA IRM Policy Manual sets forth the general principles on data standards within the Agency. This Order relates to one of several data standards used by EPA.
4. BACKGROUND.
 - a. Information technology makes efficient sharing of data among automated systems feasible, provided there exist common definitions for data elements among the systems.
 - b. The CAS Registry Number is accepted nationally and internationally as an identifier for specific, definable chemical substances.

- c. Agency programs need access to information about chemicals from other programs, agencies, States and local governments. There is a need for a chemical identification data element standard to facilitate access to chemical information.

5. POLICY.

- a. Any computer-based Agency system currently in use or being planned containing data/information on specific definable chemical substances shall contain the current CAS registry number for each chemical substance.
- b. Additional data selected from the CAS chemical registry system, such as CA Index Names and Synonyms, Molecular Formulas and the CAS Chemical Registry Records, are optional.

6. RESPONSIBILITIES.

- a. The Office of Information Resources Management (OIRM) shall:
 - (1) Provide effective leadership in developing, promulgating and enforcing this data standard.
 - (2) Provide guidance and technical assistance in implementing the requirements of this data standard.
- b. Assistant Administrators, Associate Administrators, Regional Administrators, Laboratory Directors, Headquarters Staff Office Directors, the General Counsel, the Inspector General and Senior IRM Officials shall establish procedures within their respective organizations to ensure compliance with the requirements of this data standard.
- c. The Procurement and Contracts Management Division and the Grants Administration Division shall establish procedures to ensure that contractors and assistance recipients are in compliance with the requirements of this data standard.

7. DEFINITIONS.

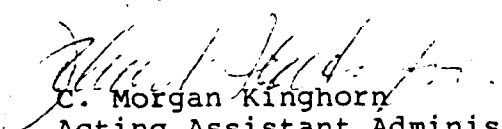
- a. "CAS Registry Number" refers to a unique, identifying number assigned by CAS to each distinct chemical substance recorded in the CAS Chemical Registry System.

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- b. "CA Index Names and Synonyms" refers to the names recorded in the CAS Chemical Registry System for each registered substance. These names include the CA Index Names and associated commercial names, author-designated names, acronyms, etc.
- c. "Molecular Formula" refers to the formula which lists the kind and number of atoms in a molecule.
- d. "CAS Unique Chemical Registry Record" refers to the machine record that represents the chemical structure in the CAS Chemical Registry System. The fundamental component is the connection table which is a detailed inventory of the atoms and bonds that comprise the two-dimensional representation of the substance's structure. Additional components of the structure record include the description of such items as stereochemistry, abnormal mass values and charges.

8. PROCEDURES.

The Information and Management Services Division of OIRM will provide any additional technical guidance for implementing the requirements of this data standard.


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for Administration and
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